Lie group techniques for Neural Learning

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Outline

- **Neural Networks**
  - a short introduction

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- **Independent Component Analysis**
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  - Constraint optimization in ICA
- **Geometric Integration of Learning equations**
  - gradient flows and algorithms on manifolds
  - MEC learning
  - Newton methods
  - diffusion algorithms

Neural Networks

Goals:

- Achieve efficient use of machines in tasks currently solved by humans
- Improve computing capabilities looking at the brain as a model
- Understand how the brain works

Applications

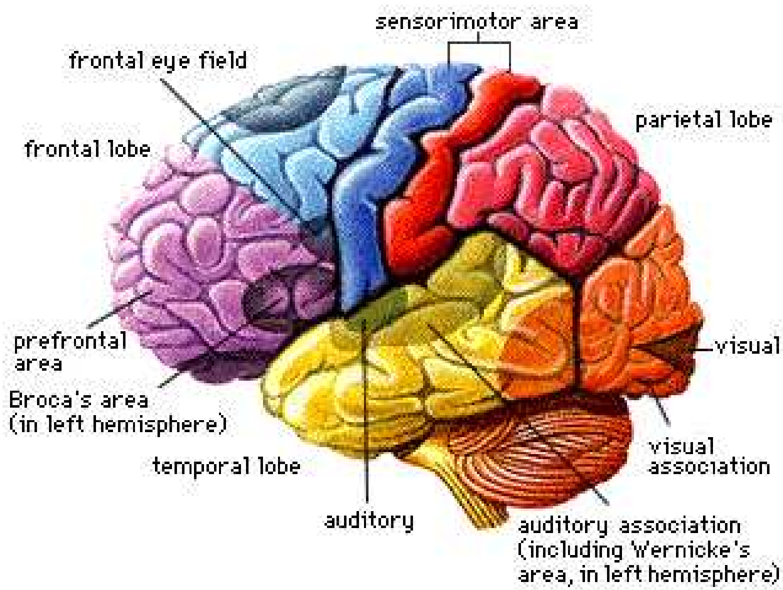
- Machine Learning
  1. How can a computer learn from a set of examples?
  2. Constraint optimization
  3. Pattern recognition, classification
  4. Associative memory
- Cognitive science
  1. Models for high level reasoning: language, problem solving
  2. Models for low level reasoning: vision, speech recognition, speech generation
- Neurobiology: find models for how the brain works

List of fields where Neural Networks are used

- Signal processing
- Control
- Robotics (navigation, vision)
- Medicine
- Business and Finance
- Data Compression

The brain as an Information Processing System

- Massively parallel: 10 billion neurons, 10000 synapses per neuron
- Slow hardware: neurons operate at about 100 Hz, while conventional CPUs execute several hundred million machine level operations per second



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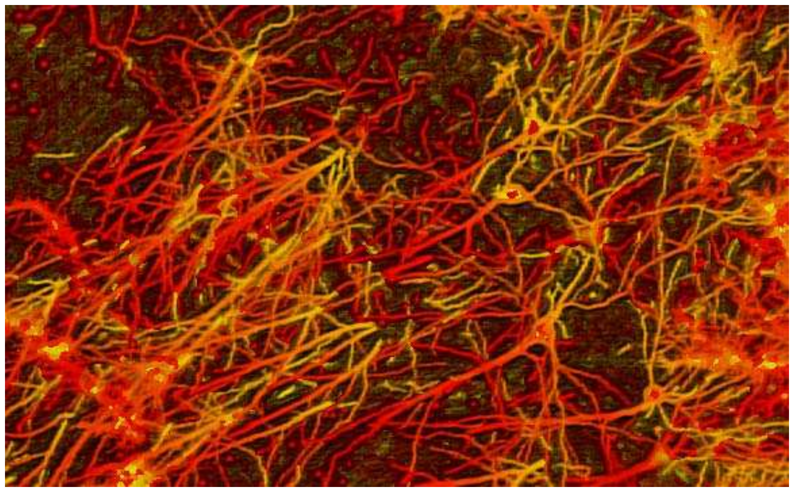

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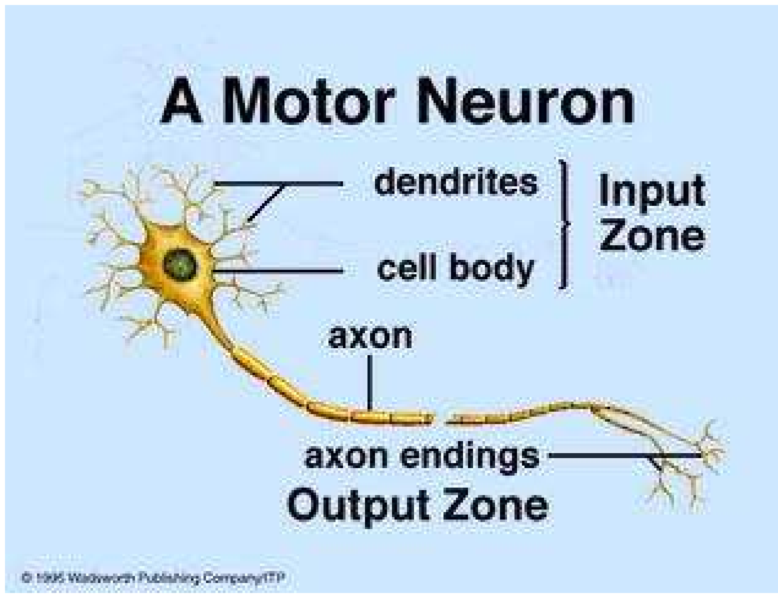
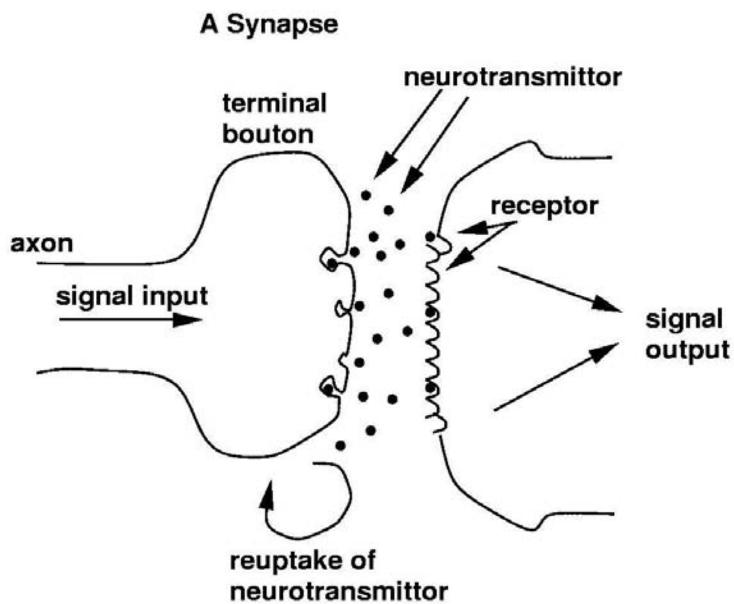


The brain as an Information Processing System

- Massively parallel: 10 billion neurons, 10000 synapses per neuron
- Slow hardware: neurons operate at about 100 Hz, while conventional CPUs execute several hundred million machine level operations per second

Synapse: transmission of a signal between neurons via a neurotransmitter. **Learning** corresponds to alteration of the strength of the connection between neurons.

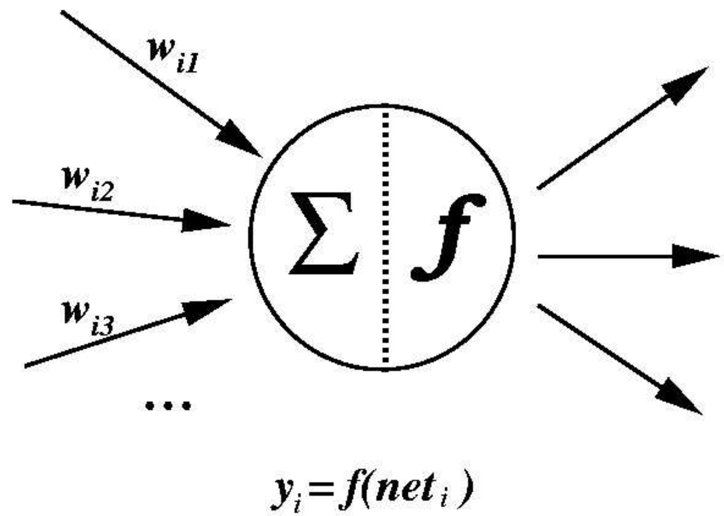


A simple model for a neuron

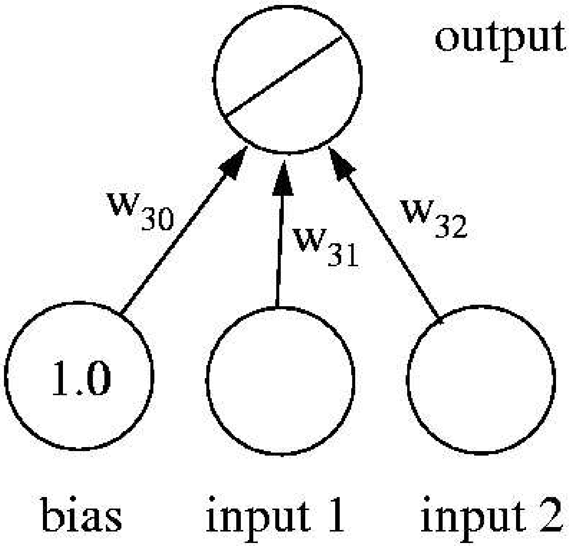
Each node (neuron) receives signal inputs form n neighbor nodes.

$$y_i = f(\sum_j w_{i,j} y_j)$$

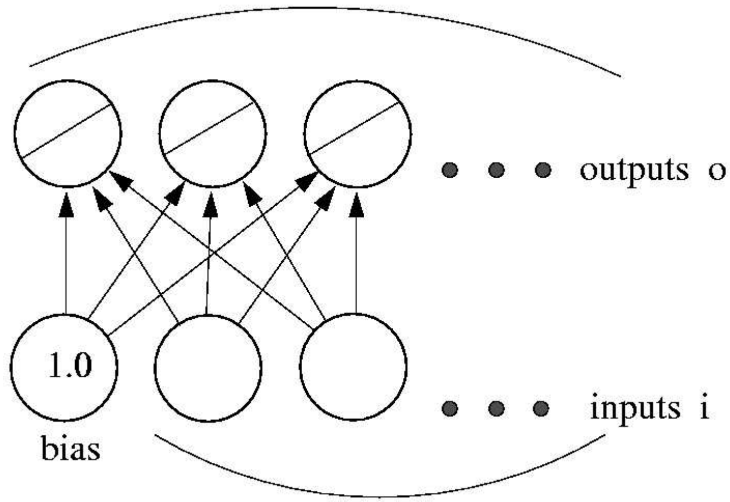
The weighted sum $\sum_j w_{i,j} y_j$ is called the net input. f is the activation function, if f is the identity we have a **linear unit**. y_i is the output signal



Linear Neural Networks



Several inputs one output



n inputs p outputs

http://www.willamette.edu/ gorr

Independent Component Analysis

The cocktail-party problem

Suppose you record two time signals $x_1(t)$ and $x_2(t)$ form two different positions in a room. Each recorded signal is a linear mixture of the voices of two speakers which emit two sources $s_1(t)$ and $s_2(t)$

$$\begin{aligned} x_1(t) &= a_{1,1}s_1(t) + a_{1,2}s_2(t) \\ x_2(t) &= a_{2,1}s_1(t) + a_{2,2}s_2(t) \end{aligned}$$

Estimate $s_1(t)$ and $s_2(t)$ from the sole knowledge of $x_1(t)$ and $x_2(t)$

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Assume the sources and the recorded signals are samples of the zero-mean random variables x_1, x_2, (**mixtures**) and s_1, s_2 (**independent components**).

Assumption $s_1(t)$ and $s_2(t)$ are statistically independent

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Assumption $s_1(t)$ and $s_2(t)$ are statistically independent

Unknown source signals $\mathbf{s}(t) = [s_1(t), \ldots, s_n(t)]^{\mathrm{T}}$
Given the output signals $\mathbf{x}(t) = A\mathbf{s}(t)$, $\mathbf{x}(t) = [x_1(t), \ldots, x_k(t)]^{\mathrm{T}}$
Unknown mixing matrix A $p \times n$

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Unknown mixing matrix A $p \times n$

Find approximations $\mathbf{y}$ of $\mathbf{s}$ by constructing a de-mixing matrix W and

$$\mathbf{y} = W\mathbf{x}.$$

Principles for reconstruction

The sum of two independent random variables usually has distribution closer to Gaussian than the two original random variables. (**Central Limit Theorem**)

$$\mathbf{x} = A\mathbf{s}$$

Find

$$\mathbf{y} = W\mathbf{x} \approx \mathbf{s}$$

maximizing nongaussianity.

A measure of nongaussianity is kurtosis,

$$\mathrm{kurt}(y) = E\{y^4\} - 3(E\{y^2\})^2,$$

with y of unit variance $\mathrm{kurt}(y) = E\{y^4\} - 3$.

Withening

Preprocessing of the output signals $\mathbf{x} \to \tilde{\mathbf{x}}$ such that the components of $\tilde{\mathbf{x}}$ are uncorrelated with variances equal to 1

$$E\{\tilde{\mathbf{x}}\tilde{\mathbf{x}}^T\} = \mathbf{I}.$$

Withening

Preprocessing of the output signals $\mathbf{x} \to \tilde{\mathbf{x}}$ such that the components of $\tilde{\mathbf{x}}$ are uncorrelated with variances equal to 1

$$E\{\tilde{\mathbf{x}}\tilde{\mathbf{x}}^T\} = \mathbf{I}.$$

Use for example $E\{\mathbf{x}\mathbf{x}^T\} = VDV^T$ and

$$\tilde{\mathbf{x}} = VD^{-1/2}V^T\mathbf{x} \;\Rightarrow\; E\{\tilde{\mathbf{x}}\tilde{\mathbf{x}}^T\} = \mathbf{I}$$

and $\tilde{\mathbf{x}} = VD^{-1/2}V^T A\mathbf{s} = \tilde{A}\mathbf{s}$, then

$$E\{\tilde{\mathbf{x}}\tilde{\mathbf{x}}^T\} = \tilde{A}E\{\mathbf{s}\mathbf{s}^T\}\tilde{A}^T = \tilde{A}\tilde{A}^T = \mathbf{I}$$

Reconstruction

Reconstruction of $\mathbf{s}$. We can look for a de-mixing matrix W s.t. $W^T W = I_p$ and $y(t) = W x(t)$ solving

$$\min_{W^T W = I_p} D(W)$$

$D(W)$ is the dependency among the components.

A. Hyvärinen and E. Oja Independent component analysis: A tutorial, *Neural Networks*.

Optimizing via gradient flows

Let $\mathcal{M}$ be a Reimannian manifold with metric $m(\cdot,\cdot)$, given $\phi : \mathcal{M} \to \mathbb{R}$ a smooth function the equilibria of

$$\dot{x}(t) = -\mathrm{grad}\phi\big(x(t)\big)$$

are the critical points of ϕ.
$\mathrm{grad}\phi$ is such that:

- $\mathrm{grad}\phi(x) \in T_x\mathcal{M}$
- $\phi'|_x\,(v) = m(\mathrm{grad}\phi(x), v)$ for all $v \in T_x\mathcal{M}$

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U. Helmke and J.B. Moore, Optimization and Dynamical Systems, Springer-Verlag 1994

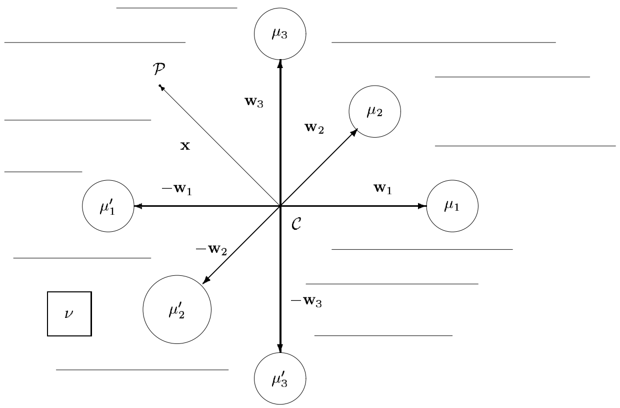
M.T. Chu and K.R. Drissel, *The projected gradient method for least squares matrix approximations with spectral constraints*, SIAM J. Num. Anal., 1990

S.I. Amari, *Natural Gradient Works Efficiently in Learning*, Neural Computation, 1998

Y. Nishimori, *Learning algorithm for ICA by geodesic flows on orthogonal* Proc. IJCNN 99

Optimizing via mechanical systems I

Consider $\mathcal{S}^* = \{[2m_i, \mathbf{w}_i]\}$ rigid system of n masses m_i with positions $\mathbf{w}_i$ (unitary distance form the origin on mutually orthogonal axis). The masses move in a viscous liquid. No translation.



$$
\begin{aligned}
\dot{W} &= HW, \quad P = -\mu HW \\
\dot{H} &= \frac{1}{4}\left[\left[F+P\right)W^T - W(F+P)^T\right]
\end{aligned}
$$

μ viscosity parameter
W matrix of the positions
H angular velocity matrix
P matrix of the viscosity resistance
F active forces

W is on $O(n)$ or on the Stiefel manifold

Optimizing via mechanical systems II

The mechanical system seen as an adapting rule for neural layers with weight matrix W.
The forces

$$F := -\frac{\partial U}{\partial W}$$

with U a **potential energy function**. The equilibria of the mechanical systems $\mathcal{S}^*$ are at the local minima of U.
Take $U = J_C$ cost function to be minimized, or $U = -J_O$ objective function to be maximized, $W(t), \;\; t \to \infty$ approaches the solution of the optimization problem.

S. Fiori, *'Mechanical' Neural Learning for Blind Source Separation*, Electronics Letters, 1999

Reformulation of the equations when $n << p$

Using the Lie algebra

$$\begin{aligned} \dot{W} &= HW, \quad P = -\mu HW \\ \dot{H} &= \tfrac{1}{4}\big[\big[F+P\big)W^T - W(F+P)^T\big] \end{aligned}$$

Using the tangent space

$$\begin{aligned} \dot{W} &= V \\ \dot{V} &= g(V,W) \end{aligned}$$

where

$$V = (GW^T - WG^T)W, \qquad G = V - W(W^T V/2 + S)$$

and

$$g(V,W) = (LW^T - WL^T)W + (GW^T - WG^T)V, \qquad L = \dot{G} - GW^T G$$

The learning algorithm

$$\begin{cases} V_{n+1} &= V_n + hg(V_n, W_n) \\ G_n &= V_n - 1/2 W_n (W_n^T V_n) \\ W_{n+1} &= \exp(h(G_n W_n^T - W_n G_n^T)) W_n \end{cases}$$

with $W_0 = I_{n \times p}$ and $V_0 = 0_{n \times p}$.
Here

$$\exp(h(G_n W_n^T - W_n G_n^T)) = [W_n, W_n^{\perp}] \exp\left(\begin{bmatrix} C - C^T & -R^T \\ R & O \end{bmatrix}\right) [W_n, W_n^{\perp}]^T$$

and $C = W_n^T G_n$, and $G_n - W_n C = W_n^{\perp} R$. We exponentiate matrices of dimension $2p \times 2p$ instead of $n \times n$.

Computational cost

For the exponential $9np^2 + np + \mathcal{O}(p^3)$ flops. For the overall geodesic learning algorithm (one step) $21np^2 + 6np + \mathcal{O}(p^3)$ flops.

Computational gain

Computing the largest eigenvalue of an $n \times n$ matrix A (discretization of the 1-D Laplacian with finite differences).

The potential energy function is $U(w) = -w^T A w$, $p = 1$.

SIZE OF A	New MEC	Old MEC
$n = 32$	4.72×10^5	1.31×10^6
$n = 64$	1.82×10^6	5.25×10^6
$n = 128$	7.39×10^6	2.10×10^7
$n = 256$	2.49×10^7	8.39×10^7

Floating point operations per iteration versus the size of the problem.

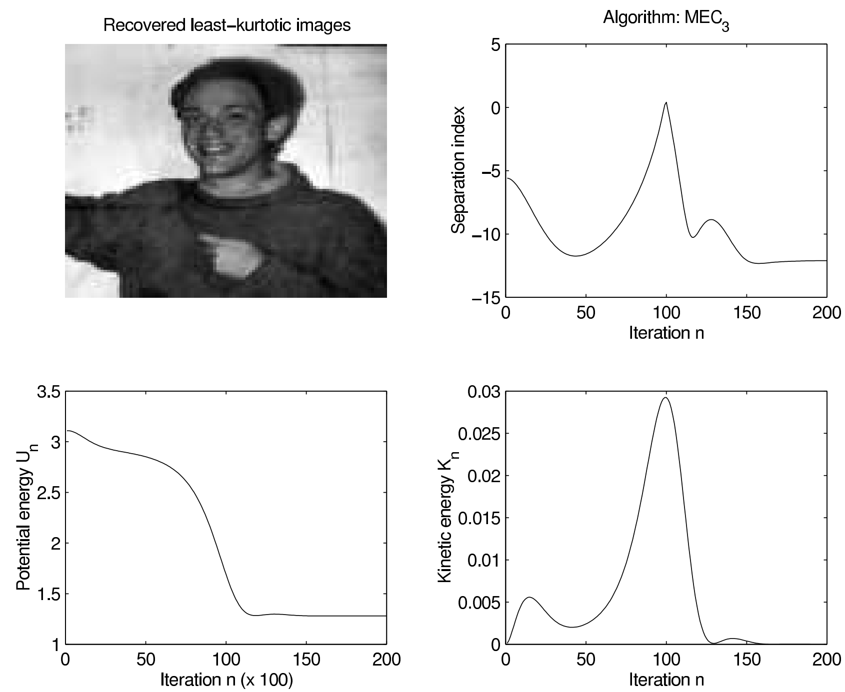
Experiments Blind source separation

Original images, with their kurtosis and their linear mixtures

Source separation

The force $F(W) = -kE_x[x(x^T W)^3_{.}]$.

Recovered image, and potential energy



References

- E. Celledoni and S. Fiori, *Neural learning by Geometric Integration of Reduced 'Rigid-Body' Equations*, J. CAM to appear.
- E. Celledoni and B. Owren, *On the implementation of Lie group methods on the Stiefel manifold*, Numerical Algorithms, 2003.

Future work

- On the orthogonal group consider quasi-geodesic paths using low-rank splittings
- Other manifolds occur in the case of multi-layer neural networks: Flag manifolds
- comparison with Newton methods

Newton methods, Mahony's approach

For finding minima or maxima of $\phi : \mathcal{G} \to \mathbb{R}$, and $\mathcal{G}$ is a Lie group,

- choose an inner product $< \cdot, \cdot >$ on the Lie algebra $\mathfrak{g}$ and take an orthonormal basis in the Lie algebra $X_1, \ldots, X_d$, and $\tilde{X}_1, \ldots, \tilde{X}_d$ the right invariant vector fields
- $$\mathrm{grad}\phi = \sum_{i=1}^{d} m(\tilde{X}_i, \mathrm{grad}\phi)\tilde{X}_i = \sum_{i=1}^{d} (\tilde{X}_i\phi)\tilde{X}_i$$

  ($m(\tilde{X}, \tilde{Y}) =< X, Y >$ (right invariant group metric))
- if $\exp(X)\sigma$ is a critical point of ϕ, the vector field $\tilde{X}$ satisfies,

$$\mathrm{grad}\phi(\sigma) + \mathrm{grad}(\tilde{X}\phi)(\sigma) = 0$$

R. E. Mahony *The constrained Newton method on a Lie group and the symmetric eigenvalue problem* , Lin. Alg. and Appl. 1996

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  ($m(\tilde{X}, \tilde{Y}) =< X, Y >$ (right invariant group metric))
- Find X^k such that $\tilde{X}^k$ solves

  $$\mathrm{grad}\phi(\sigma_k) + \mathrm{grad}(\tilde{X}^k \phi)(\sigma_k) = 0$$

  set $\sigma_{k+1} = \exp(X^k)\sigma_k$, $k \leftarrow k+1$ and continue, (equivalent to Lie Euler for $\dot{\sigma} = X^k \sigma$, $\sigma(0) = \sigma^k$)

R. E. Mahony *The constrained Newton method on a Lie group and the symmetric eigenvalue problem* , Lin. Alg. and Appl. 1996

Newton methods, other approaches

- A. Edelman, T. Arias, S.T. Smith, *The geometry of Algorithms with orthogonality constrains*, SIAM J. Matrix Anal. Newton methods and Conjugate Gradient on the Stiefel and Grassman manifolds.
- B. Owren and B. Welfert, *The Newton iteration on Lie groups*, BIT 2000. Context: implicit Lie group methods, this method can be applied directly in the implicit integration of gradient flows
- L. Lopez, C. Mastroserio, T. Politi. *Newton-type methods for solving nonlinear equations on quadratic matrix groups.* J. CAM 2000. Similar as previous one, using the Cayley transformation
- J.P. Dedieu and D. Nowicki, *Symplectic methods for the approximation of the exponential and the Newton sequence on Reimannian submanifolds*, Preprint february 2004. General Reimanninan manifold, use of tangent space parametrizations, geodesic seen as the trajectory of a free particle attached to the manifold

Diffusion-type algorithms

Perturbation of the standard Reimannian gradient to obtain a rondomized gradient. Diffusion-type gradient on $\mathfrak{SO}(n)$

$$V_{\mathrm{diff}}(t) = V(t) + \sqrt{2\theta} \sum_{k=1}^{n(n-1)/2} X_k \frac{d\mathcal{W}_k}{dt}$$

$V(t)$ deterministic gradient, X_k is a basis of the Lie algebra $\mathfrak{so}(n)$ orthogonal with respect to the chosen metric, and $\mathcal{W}_k(t)$ are real-valued, independent standard Wiener processes i.e. a random variable $\mathcal{W}$ continuous in t s.t.

- $\mathcal{W}(0) = 0$ with probability 1
- for $0 \leq \tau < t$ the random variable $\mathcal{W}(t) - \mathcal{W}(\tau)$ is normally distributed with mean zero and variance $t - \tau$
- for $0 \leq \tau < t < u < v$, the increments $\mathcal{W}(t) - \mathcal{W}(\tau)$ and $\mathcal{W}(v) - \mathcal{W}(u)$ are statistically independent

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$V(t)$ deterministic gradient, X_k is a basis of the Lie algebra $\mathfrak{SO}(n)$ orthogonal with respect to the chosen metric, and $\mathcal{W}_k(t)$ are real-valued, independent standard Wiener processes The learning differential equation is

$$\frac{dW}{dt} = -V_{\text{diff}}(t))W$$

Langevin-type stochastic differential equation on the orthogonal group

X. Liu, A. Srivastava, K. Galivan, *Optimal linear representation of images for object recognition*, IEEE Trans. Pattern Analysis, 2004.

Conclusion

- Integration of learning equations and gradient flows is achieved with simple first order explicit Lie group integrators
- Efficient approximation of the matrix exponential from a Lie algebra to a Lie group or the computation of geodesics is crucial
- Development of methods based on other coordinate maps then the exponential, and quasi-geodesic strategies
- Geometric integration of stochastic differential equations